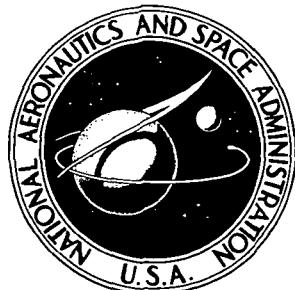


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FIGURE-OF-MERIT CALCULATION METHODS FOR ORGANIC HEAT-PIPE FLUIDS

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SUMMARY

With only chemical formulas and operating temperatures specified, selected correlating equations and tables of chemistry-effect functions allow estimates of figures of merit for organic heat-pipe fluids.

INTRODUCTION: SELECTING ORGANIC HEAT-PIPE FLUIDS

Some organic chemicals perform adequately as heat-pipe fluids and offer special application advantages (refs. 1 to 3). The heat-pipe potentialities of such compounds depend on their properties as indicated by the simple figures of merit described in reference 4:

"zero-g figure of merit" or "liquid transport factor":

$$L = \frac{\sigma_l \rho_l \lambda_l}{\mu_l} \quad (1)$$

"g-field figure of merit":

$$G = \frac{\sigma_l}{\rho_l} \quad (2)$$

"nucleation tolerance factor":

$$N = \frac{k_l \sigma_l}{\lambda_l \rho_v} \quad (3)$$

where σ_l is surface tension, ρ_l is density, λ_l is latent heat of vaporization, μ_l is viscosity, k_l is thermal conductivity - all of the liquid; and ρ_v is saturated-vapor density.

Equations (1) to (3) are convenient for screening heat-pipe fluids. However, tabulations of the properties necessary to compute these figures of merit over wide temperature variations are often unavailable for less common organic compounds. Fortunately references 5 and 6 provide correlations collected from numerous sources to predict physical characteristics of various chemicals as functions of molecular formulas and operating temperatures only. So this minimal information allows estimations and comparisons of heat-pipe figures of merit for organic fluids. The present report comprises selections of appropriate equations, conversions, and chemistry-effect functions to enable such screening.

CALCULATION METHODS: PHYSICAL PROPERTIES AND FIGURES OF MERIT

Unless otherwise indicated input variables and results of the following equations bear international units (SI, mksa). Using this system required numerous conversions in the physical-property correlations, which come from long-established chemical-engineering references (refs. 5 and 6). And because these expressions relate to chemistry and thermodynamics, the concept of the mol naturally arises: the cgs gram-mol, the British pound-mol, but the mksa gram-mol (ref. 7) not the mksa kilogram-mol. So the molecular weight M appears here as grams per gram-mol. This detail is, of course, very important in preventing thousandfold errors during kilogram transformations of the many mol-based characteristics.

Except M and the gas constant R ($8.314 \text{ J(K}^{-1}\text{)(mol}^{-1}\text{)}$), though, the dimensions of the physical properties in this report involve only the usual mksa units (C_p , $(\text{J})(\text{kg}^{-1})\text{(K}^{-1}\text{)}$; k , $(\text{J})(\text{m}^{-1})(\text{sec}^{-1})(\text{K}^{-1})$; P , $(\text{N})(\text{m}^{-2})$; T , K ; λ , $(\text{J})(\text{kg}^{-1})$; μ , $(\text{N})(\text{sec})(\text{m}^{-2})$; ρ , $(\text{kg})(\text{m}^{-3})$; and σ , $(\text{N})(\text{m}^{-1})$). The appendix defines the symbols, and reference 5 gives unconverted versions of equations (4) to (23).

INPUT VARIABLES

Computing figures of merit for an organic heat-pipe fluid begins with specification of the chemical formula (CF) and the operating temperature T_l of the liquid. Usually the normal boiling point T_b is also available through the literature or simple testing. And because correlations leading to k_l , λ_l , μ_l , σ_l , ρ_l , and ρ_v depend strongly on T_b a well-determined value of this variable is desirable. But if such a T_b is lacking, the first equation of the next section yields a reasonable estimate.

NORMAL-BOILING AND CRITICAL POINTS

Equations for normal-boiling and critical points are given in this section.

Normal boiling temperature:

$$T_b = \frac{637 [R_D]^{1.47} + B}{[P]} \quad (4)$$

The parachor $[P]$ and molar refraction $[R_D]$ are sums of CF effects taken directly from table 3-285 of reference 5 (or table 3-287 for $[P]$). And B is a chemistry-dependent constant from table 3-286.

Critical-point temperature and pressure:

$$T_c = \frac{T_b}{\frac{\Sigma \Delta_T}{100}} \quad (5)$$

$$P_c = \frac{1.013 \times 10^9 M}{(\Sigma \Delta_P)^2} \quad (6)$$

Here again $\Sigma \Delta_T$ and $\Sigma \Delta_P$ result from summations of CF contributions listed in tables 3-288 and 3-289 of reference 5.

Normal-boiling-point latent heat of vaporization:

$$\lambda_b = \frac{RT_c T_b \ln \frac{P_c}{1.013 \times 10^5}}{(T_c - T_b)M \times 10^{-3}} \quad (7)$$

Critical-point compressibility factor and density:

$$Z_c = \frac{1}{3.43 + 0.0067 \left(\frac{\lambda_b M}{4.184 \times 10^6} \right)^2} \quad (8)$$

$$\rho_c = \frac{P_c}{Z_c R T_c} M \times 10^{-3} \quad (9)$$

Normal-boiling-point liquid density:

$$\rho_{l,b} = \rho_c \left(1.981 + 0.422 \log \frac{P_c}{1.013 \times 10^5} \right) \quad (10)$$

Having these normal-boiling and critical characteristics enables the following evaluations of physical properties necessary to compute the heat-pipe figures of merit.

SATURATED-FLUID PROPERTIES AT LIQUID OPERATING TEMPERATURE

Saturated-fluid properties at liquid operating temperatures are given in this section.

Saturated-vapor pressure and density:

$$P_v = P_c \left(\frac{T_l}{T_c} \right)^{\alpha'} \times 10^{(0.137 - 0.0364\alpha')B'} \quad (11)$$

where

$$B' = 36 \frac{T_c}{T_l} - 35 - \left(\frac{T_l}{T_c} \right)^6 + 42 \ln \frac{T_l}{T_c} \quad (12)$$

and

$$\alpha' = 0.878 + 2.11 \frac{\log \frac{P_c}{1.013 \times 10^5}}{\frac{T_c}{T_b} - 1} \quad (13)$$

The compressibility factor Z_v is now required to obtain the saturated-vapor density ρ_v from the corresponding pressure P_v and temperature T_l . Table I worked up from data presented in reference 6 allows interpolations of Z_v as a function of Z_c , $T_{l,r} = T_l/T_c$, and $P_{v,r} = P_v/P_c$. Then

$$\rho_v = \frac{P_v M \times 10^{-3}}{Z_v R T_l} \quad (14)$$

Liquid density:

$$\rho_l = (\rho_{l,b} - \rho_{v,b}) \left(\frac{T_c - T_l}{T_c - T_b} \right)^{1/3} + \rho_v \quad (15)$$

The saturated-vapor density at the normal boiling point $\rho_{v,b}$ results from equation (14) and the preceding paragraph used with T_b and $P_{v,b} = 101325$ newtons per square meter.

Surface tension:

$$\sigma_l = \left[\frac{[P](\rho_l - \rho_v)}{M} \right]^4 \times 10^{-15} \quad (16)$$

For this equation a summation of CF effects taken from table 3-294 of reference 5 produces the parachor $[P]$.

Latent heat of vaporization:

$$\lambda_l = \frac{RT_c T_b}{M \times 10^{-3}} \left(\ln \frac{P_c}{1.013 \times 10^5} \right) \frac{(T_c - T_l)^{0.38}}{(T_c - T_b)^{1.38}} \quad (17)$$

Constant-pressure specific heat and thermal conductivity:

$$C_{p,l} = C_{p,l,20} \left(\frac{1 - \frac{140.7}{T_c}}{1 - 0.48 \frac{T_l}{T_c}} \right)^{2.8} \quad (18)$$

Summing CF contributions from table 3-291 of reference 5 and multiplying by $4184/M$ give the liquid specific heat at 20°C to be used in equation (18). With the resulting $C_{p,l}$,

$$k_l = \frac{4.27 C_{p,l} \rho_l^{4/3}}{\alpha M^{1/3}} \times 10^{-8} \quad (19)$$

where

$$\alpha = \alpha_{30} - (\alpha_{30} - 1) \left[\frac{T_c - T_l}{T_c - 303.15 \left(\text{or } \frac{T_c}{2} \right)} \right] = \frac{\lambda_b M}{T_b \times 8.8 \times 10^4} \left[\frac{T_l - 303.15 \left(\text{or } \frac{T_c}{2} \right)}{T_c - 303.15 \left(\text{or } \frac{T_c}{2} \right)} \right] + \frac{T_c - T_l}{T_c - 303.15 \left(\text{or } \frac{T_c}{2} \right)} \quad (20)$$

unless this value is less than unity; then $\alpha = 1.0$ is used. And

$$\alpha_{30} = \frac{\lambda_b M}{T_b \times 8.8 \times 10^4} \quad (21)$$

according to reference 5, which indicates that this constant applies "at 30° C for most liquids or at $T_c/2$ for low boilers such as methane, N₂, and ethylene Calculated values of $\alpha < 1$ should be taken as unity, and at temperatures other than 30° C (or $T_c/2$), α may be assumed to vary linearly between values given by the Eq. [(21)] at 30° C and 1.0 at T_c . "

Liquid viscosity:

$$\mu_l = 1.167 \rho_l^{1/2} \times 10^{B'' \left(\frac{T_c}{T_l} - 1 \right) - \frac{11}{2}} \quad (22)$$

where B'' is another sum of CF effects from table 3-297 of reference 5.

FIGURES OF MERIT

Substituting fluid-property values from the equations of the preceding section into equations (1) to (3) yields figures of merit for organic heat-pipe fluids:

$$L = \frac{\sigma_l \rho_l \lambda_l}{\mu_l} = \frac{(16)(15)(17)}{(22)} \quad (1')$$

$$G = \frac{\sigma_l}{\rho_l} = \frac{(16)}{(15)} \quad (2')$$

$$N = \frac{k_l \sigma_l}{\lambda_l \rho_l} = \frac{(19)(16)}{(17)(14)} \quad (3')$$

DISCUSSION: USE OF CALCULATED FLUID PROPERTIES AND FIGURES OF MERIT

The selected correlations for physical properties involve generally modest average errors, which references 5 and 6 discuss. But the question of accuracy is a moot one

since these expressions are of value only in the absence of the necessary compilations of experimental data.

When such collections of physical properties are unavailable, an initial screening with only L (eq. (1')) and G (eq. (2')) estimates seems appropriate for conventional heat pipes. Then N (eq. (3')) comparisons for the more promising fluids would further reduce the field. This is a desirable approach because L is the most widely used figure of merit, because G bolsters the meaning of L and depends only on results necessary to compute L , and because k_l and ρ_v required for N involve time-consuming calculations.

Neglecting ρ_v at the outset simplifies the calculations of ρ_l (eq. (15)) and σ_l (eq. (16)) and limits the initial screening to heat pipes where $\rho_v \ll \rho_l$. But this condition generally applies because the liquid pumping potential σ_l (eq. (16)) decreases very rapidly as $\rho \rightarrow \rho_v$.

Incidentally, the ratio form for the correlation of density differences

$$\frac{\rho_l - \rho_v}{\rho_{l,b} - \rho_{v,b}} = \left(\frac{T_c - T_l}{T_c - T_b} \right)^{1/3} \quad (15')$$

is quite similar to that for latent heats of vaporization:

$$\frac{\lambda_l}{\lambda_b} = \left(\frac{T_c - T_l}{T_c - T_b} \right)^{0.38} \quad (23)$$

This comparison indicates clearly that the heat pipe becomes less effective as the density of the vapor increases toward that of the liquid - because simultaneously the heat of vaporization approaches zero. So heat pipes, which essentially transport the enthalpy of condensation, should operate with $\rho_v \ll \rho_l$. Consequently, neglecting ρ_v effects in the suggested initial screening is a justifiable economy.

These simplifications used with the selected physical-property correlations and the figure-of-merit expressions allow meaningful first-round evaluations of unusual organic heat-pipe fluids.

Lewis Research Center,

National Aeronautics and Space Administration,

Cleveland, Ohio, September 18, 1973,

503-25.

APPENDIX - SYMBOLS

B	CF-dependent constant
B'	function of reduced temperature T_l/T_c in vapor-pressure equation
B''	sum of CF effects in liquid-viscosity equation
$C_{p,l}$	constant-pressure specific heat for liquid
$C_{p,l,20}$	constant-pressure specific heat for 20° C liquid
G	G-field figure of merit
k_l	thermal conductivity of liquid
L	liquid transport factor (zero-g figure of merit)
M	molecular weight
N	nucleation tolerance factor
[P]	parachor, sum of CF effects in normal-boiling-temperature and surface-tension equations
P_c	pressure at critical point
P_v	saturated-vapor pressure at T_l
$P_{v,b}$	saturated-vapor pressure at normal boiling point
R	gas constant
[R_D]	molar retraction, sum of CF effects in normal-boiling-temperature equation
T_b	normal-boiling temperature
T_c	critical-point temperature
T_l	liquid operating temperature
Z_c	critical-point compressibility factor
Z_v	compressibility factor of saturated vapor at T_l
α	functional factor in thermal-conductivity equation
α_{30}	functional factor at 30° C (or $T_c/2$) in thermal-conductivity equation
α'	functional factor in exponents of vapor-pressure equation
λ_b	latent heat of vaporization at normal boiling point
λ_l	latent heat of vaporization at T_l
μ_l	liquid viscosity at T_l
ρ_c	critical-point density

ρ_l	liquid density at T_l
$\rho_{l,b}$	liquid density at normal boiling point
ρ_v	saturated-vapor density at T_l
$\rho_{v,b}$	saturated-vapor density at normal boiling point
$\Sigma\Delta_p$	sum of CF effects in critical-point-pressure equation
$\Sigma\Delta_T$	sum of CF effects in critical-point-temperature equation
σ_l	liquid surface tension at T_l

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TABLE I. - COMPRESSIBILITY FACTORS FOR SATURATED VAPORS

		Critical-point compressibility factor, Z_c							
		0.23		0.25		0.27		0.29	
Reduced saturated- vapor pres- sure at T_l' , $P_{v,r} = P_v/P_c$	Reduced liquid operating temperature, $T_{l,r} = T_l/T_c$	Compressibility factor of satu- rated vapor at $T_l',$ Z_v		Reduced liquid operating temperature, $T_{l,r} = T_l/T_c$		Compressibility factor of satu- rated vapor at $T_l',$ Z_v		Reduced liquid operating temperature, $T_{l,r} = T_l/T_c$	
		$T_{l,r}$	Z_v	$T_{l,r}$	Z_v	$T_{l,r}$	Z_v	$T_{l,r}$	Z_v
0.1	0.769	0.872	0.759	0.893	0.738	0.901	0.712	0.902	
.2	.825	.810	.816	.830	.802	.837	.777	.839	
.3	.863	.752	.856	.872	.845	.781	.827	.783	
.4	.891	.700	.884	.727	.876	.738	.862	.742	
.6	.937	.593	.932	.623	.927	.633	.919	.644	
.8	.971	.480	.970	.505	.968	.521	.963	.533	
.9	.986	.405	.986	.426	.984	.443	.982	.461	
1.0	1.000	.230	1.000	.250	1.000	.270	1.000	.290	

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